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Characterizing Solute Drag on Perfect and Extended Dislocations

RYAN B. SILLS[1,2] AND WEI CAI[1]

[1]MECHANICAL ENGINEERING, STANFORD UNIVERSITY

[2]SANDIA NATIONAL LABORATORIES, LIVERMORE, CA

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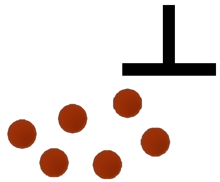
Overview

- Nature of solute drag
- Numerical drag calculation
- Results

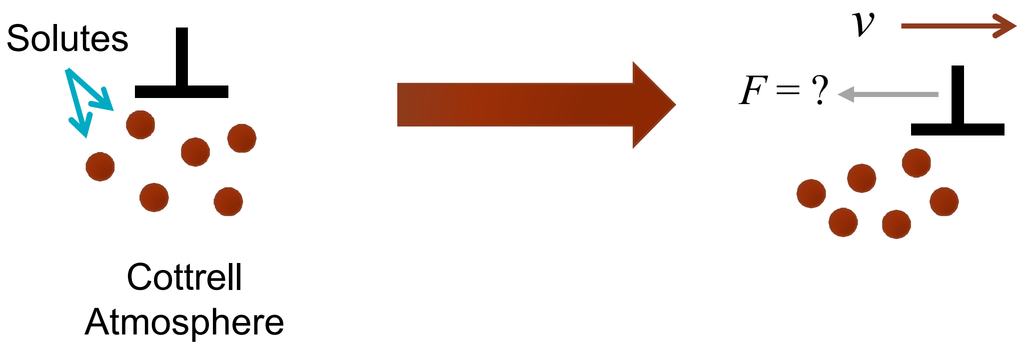
Nature of solute drag



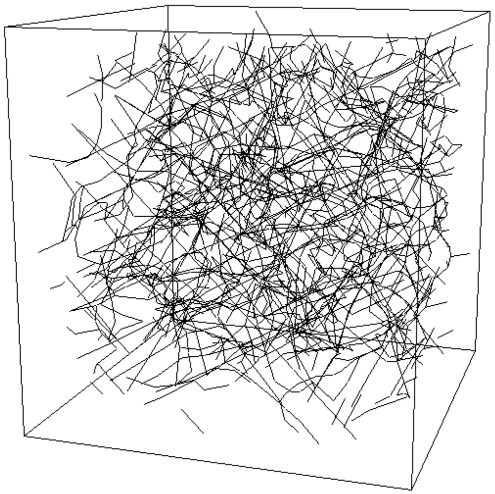
Cottrell atmosphere and solute drag

Solid solutions are ubiquitous in metallic systems

- Alloying
- Contaminants (e.g. hydrogen)



Including solute drag in dislocation dynamics



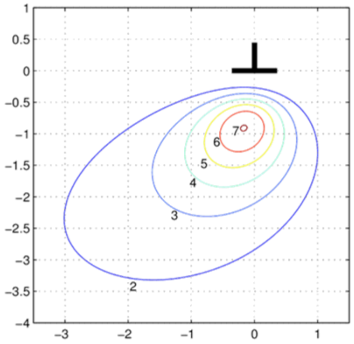
- Interested in large-scale simulations
- Full simulation of solute field not feasible
  - › Very fine computational grid required
- Our approach: Use mobility law to incorporate drag effects

$$\mathbf{F}_{\mathrm{drag}}(\mathbf{v}) = \mathbf{F}_{\mathrm{drive}} \quad \Longrightarrow \quad \mathbf{v} = \mathbf{M}(\mathbf{F}_{\mathrm{drive}})$$

Mobility Law (for $\mathbf{M}$)

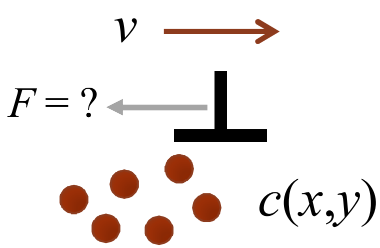
→ Need to determine $\mathbf{F}_{\mathrm{drag}}(\mathbf{v})$

Numerical drag calculation



Cottrell and Jaswon (1949)
Yoshinaga and Morozumi (1971)
Takeuchi and Argon (1979)
James and Barnett (1985)
Hirth and Lothe (1982)
Fuentes-Samaniego et *al*. (1984)
Zhang and Curtin (2008)

Steady-state drag calculation



Focus on achieving convergent solution

- Enabled by non-singular dislocation theory (Cai et *al*., 2006)

Consider extended dislocations

Solute concentration field calculation

$$\frac{\partial c}{\partial t} = -\nabla \cdot \mathbf{J} = 0 \qquad \text{(steady state)}$$

Finite difference and solve with Newton's method

Drag force calculation

$$\sigma_{xy} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} [c(x',y') - c_0]\, \sigma_{xy}^{\text{solute}}(x_c - x', y_c - y')dx'dy'$$

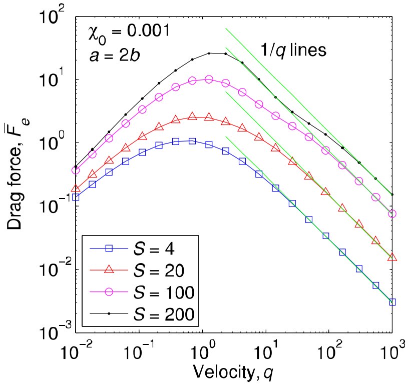
Background concentration (c_0)

Stress field of a solute ($\sigma_{xy}^{\text{solute}}$)

Evaluate with adaptive quadrature in MATLAB

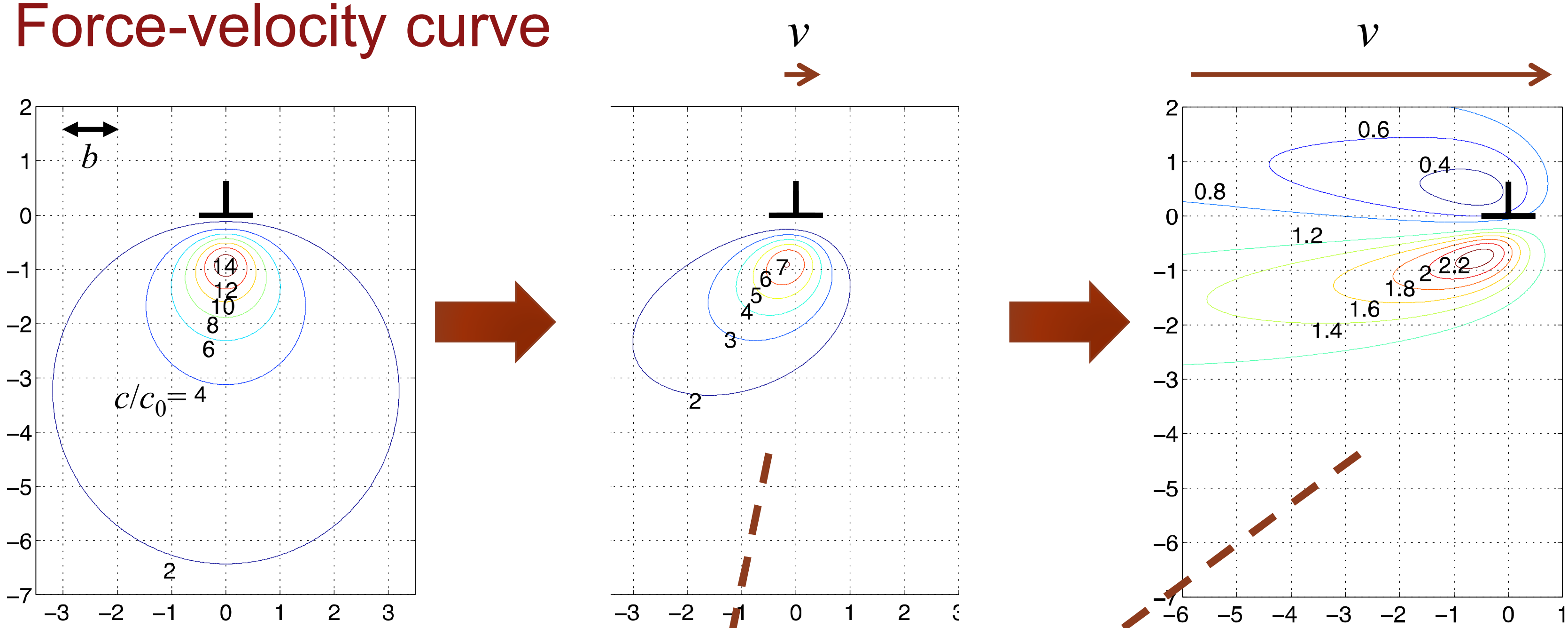
$$F = \sigma_{xy} b$$

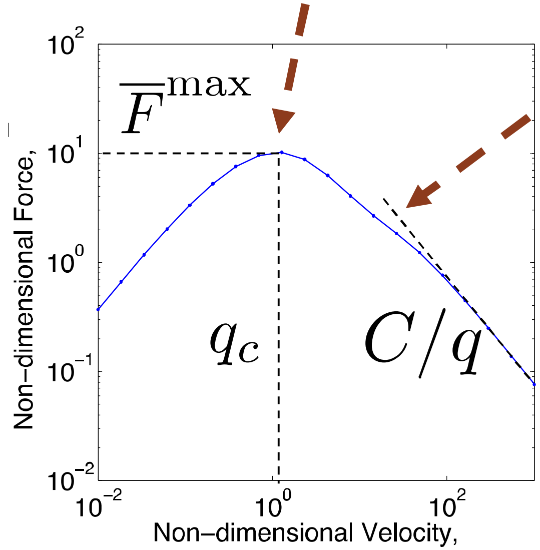
Results



χ_0 = 0.001
$a = 2b$
1/q lines
Drag force, $\bar{F}_e$
Velocity, q
S = 4
S = 20
S = 100
S = 200

Force-velocity curve

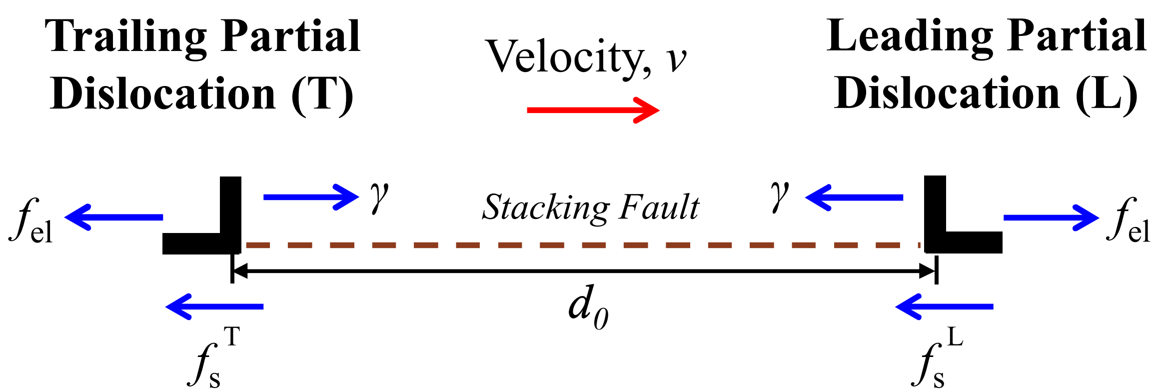




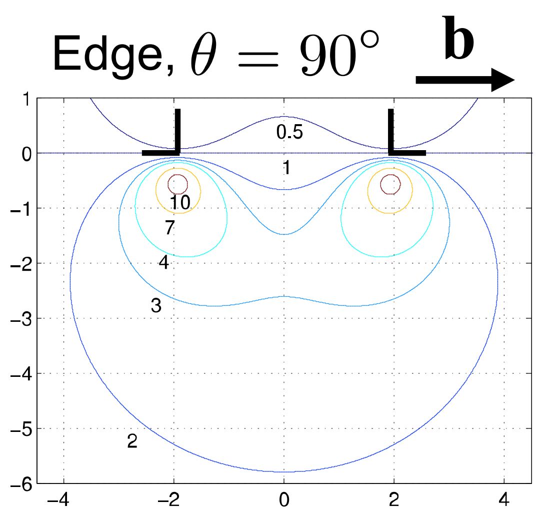
$$\overline{F} = \overline{F}\left(q, c_0, S, \theta, \frac{\hat{\gamma}}{\mu b}, \frac{a}{b}\right)$$

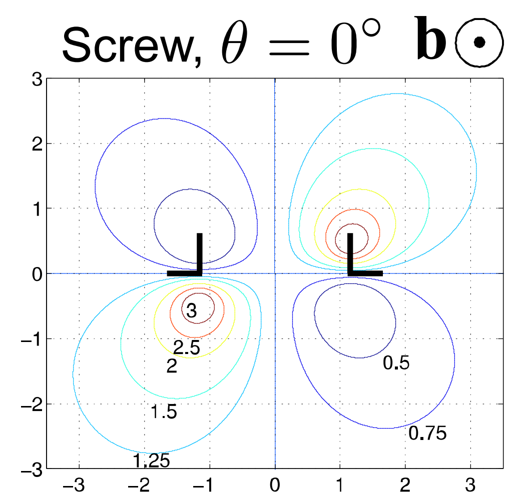
Non-dimensional Force Expression

Extended dislocations – Partial separation distance



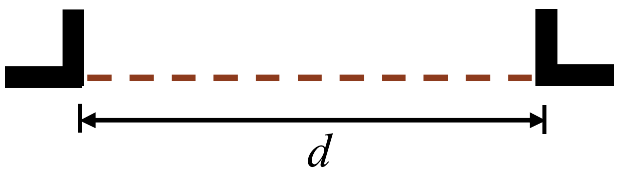
$$f_s^T(d) - f_s^L(d) = 2[f_{el}(d_0) - f_{el}(d)]$$





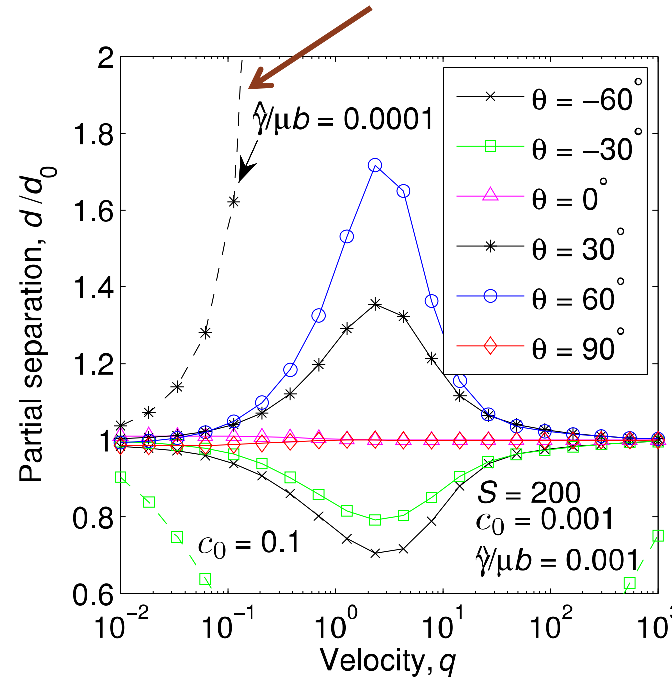
Extended edges experience 4x more drag than extended screws

Extended dislocation results



$d_0 =$ Solute-free separation distance

Separation distance goes to infinity!



- Deformation twinning in low SFE metals possibly promoted by solutes
  - Stainless steel with H (San Marchi et *al*., 2011)
  - Stainless steel with N (Mullner et *al*. 1993)

Summary

- Analytical form for force-velocity curve and DD mobility law

$$\overline{F}(q) = \frac{Cq}{q^2 + \left(C/\overline{F}^{\max} - 2q_c\right) q + q_c^2}$$

  - Can incorporate solute drag in DD simulations

- Extended screws see 75% less drag than extended edges

- Atmosphere can change partial separation significantly
  - Independent of changes in SFE

- Manuscript in-preparation
  - *Solute drag on perfect and extended dislocations*, R. B. Sills and W. Cai